Isoamyl ether

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 137

Global applicability domain: Inside

Local applicability domain index: 6.37e-01

Confidence level: 6.20e-01

Nearest Neighbors from the Training Set

Image not found
Isoamyl ether
Measured: 170
Predicted: 137

Image not found
Menthol
Measured: 10.8
Predicted: 23.5

Image not found
(1R,2S,5R)-(-)-Menthol
Measured: 10.8
Predicted: 23.5

Image not found
N,N-Diethylaniline
Measured: 102
Predicted: 12.8

Image not found
1-Ethenoxy-2-ethylhexane
Measured: 603
Predicted: 284

Image not found
1-Naphthalenamine, N-ethyl-
Measured: 209
Predicted: 47.9